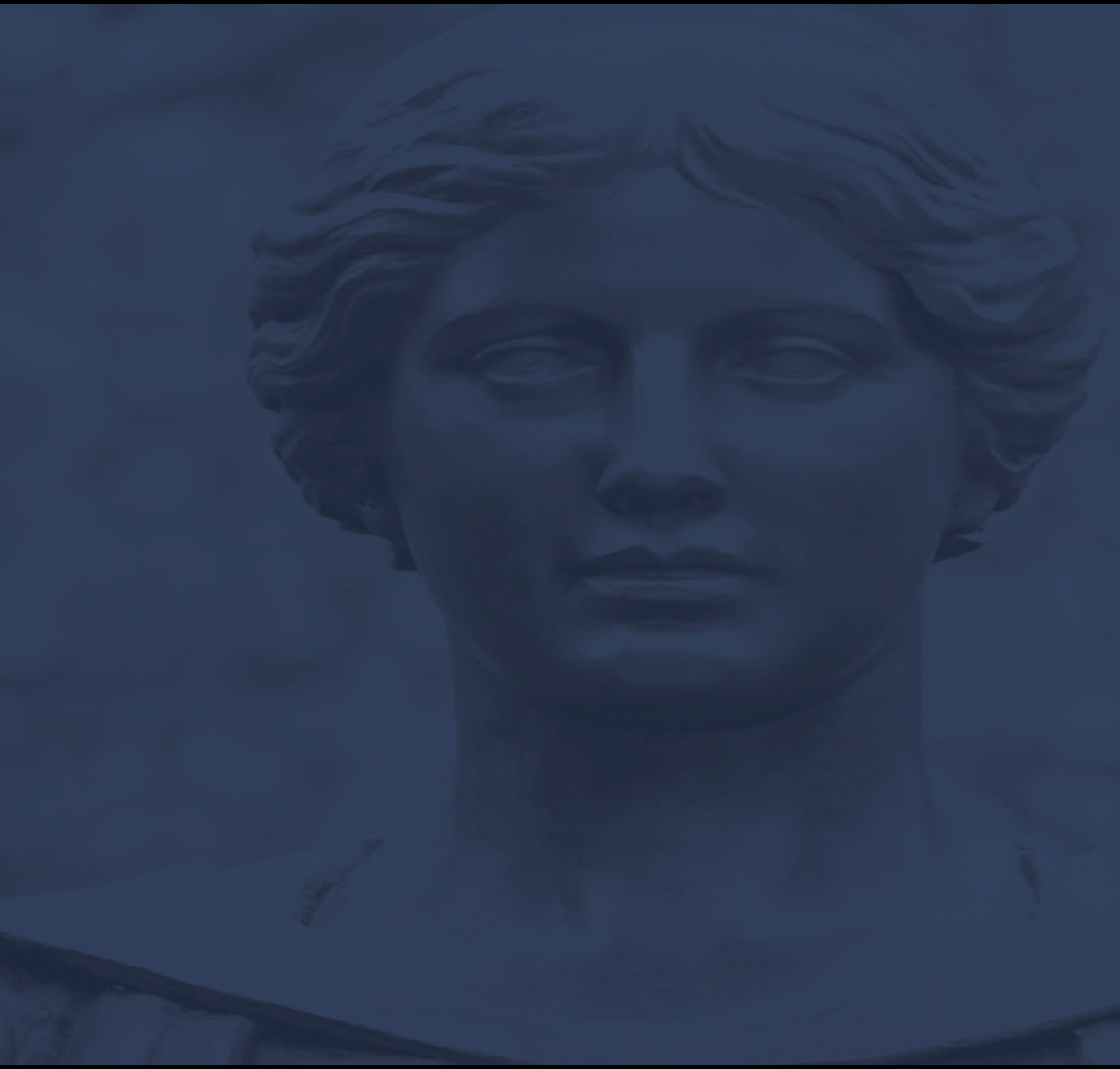
ILLINOIS



Machine Learning in Material Design

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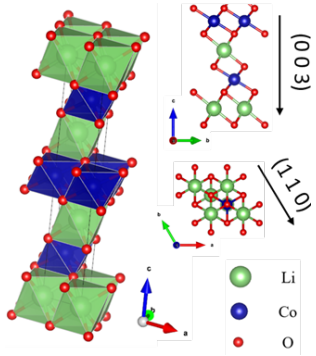
Generic process of building a ML model

Physics-informed machine learning

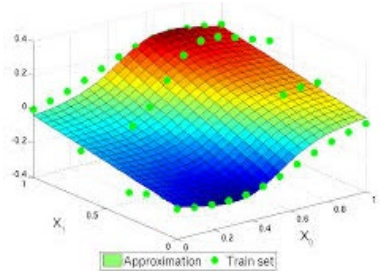
Physical prior knowledge + Data

Dataset construction

Featurization/ Encoding



Training/Optimization

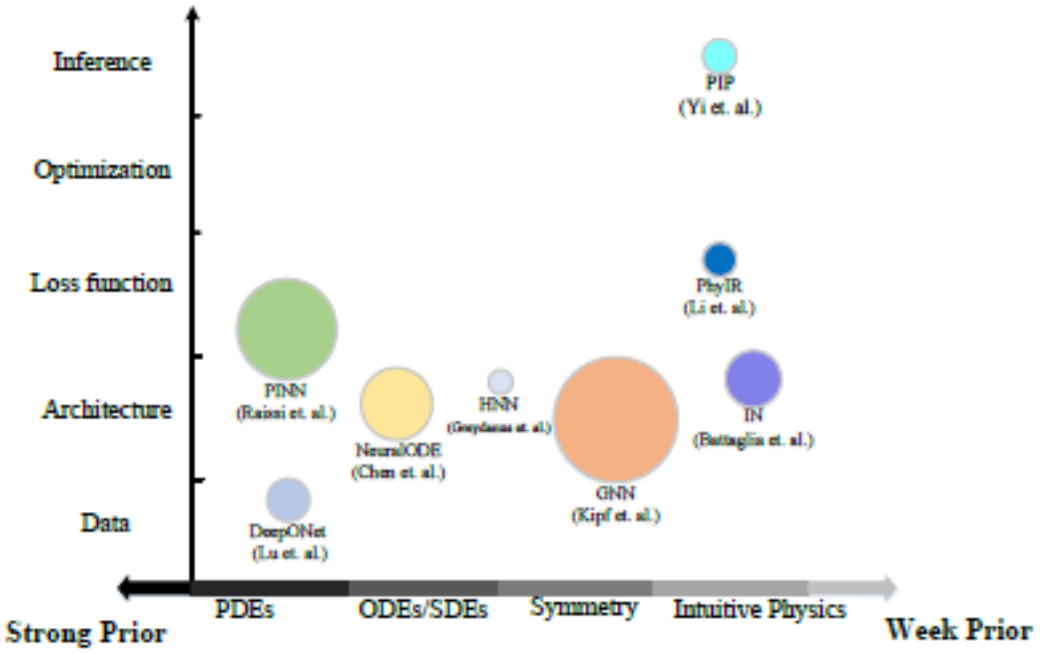


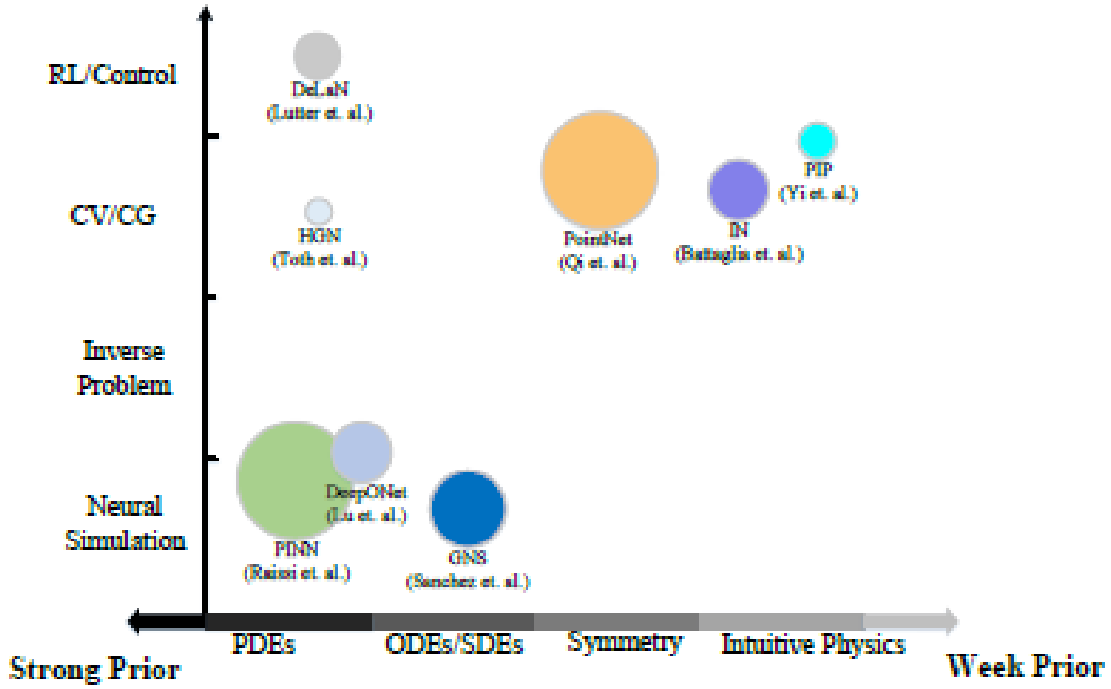
Evaluation

Physics-informed machine learning

- There are significant limitations when deploying data-driven models in real-world applications.
  - Lack of robustness
  - Hard to interpretate
  - Struggle to conform physical constraints or commonsense reasoning
  - Suboptimal performance outside of the training distribution
- These issues are particularly pertinent in scientific problems where data often tends to be sparse and noisy due to the high cost and the presence of environmental and device-related noise.
- To address the challenges, numerous methods have been proposed by researchers to integrate physical knowledge and data with machine learning.

Physics-informed machine learning





Physics prior

- Physical prior knowledge refers to the understanding of the fundamental laws and principles of physics that describe the behaviors of the physical world.
  - Partial differential equations (PEDs)
  - Symmetry constraints
  - Intuitive physical constraints
- Differential equations including partial differential equations, ordinary differential equations and stochastic differential equations represent precise physical laws that can effectively describe various scientific phenomena based on assumptions.

Physics prior

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Heat Transfer: $$\frac{\partial}{\partial x}\left(\frac{k\partial T}{\partial x}\right)+\frac{\partial}{\partial y}\left(\frac{k\partial T}{\partial y}\right)+\frac{\partial}{\partial z}\left(\frac{k\partial T}{\partial z}\right)+q_v=\rho C_p\frac{\partial T}{\partial t}$$

Force equilibrium equation: $$\frac{\partial \sigma_{jk}}{\partial x_j}+b_k=0 \quad k=1,2,3$$

Physics prior

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  - Intuitive physical constraints
- Symmetry constraints are considered a weak inductive bias compared to PDEs and ODEs. Examples of symmetry constraints are translation, rotation, and permutation invariance or equivariance.
- Intuitive physics refers to the common-sense knowledge about the physical world that humans possess. Examples include gravity and conservation laws.

How to integrate physical priors

- The incorporation of physical prior knowledge can be achieved through modifications to the foundational components in developing machine learning models including data, model architecture, loss functions, optimization algorithm and inference.
  - Data: we could augment or process the dataset utilizing available physical prior like symmetry.
  - Model: we could embed physical prior into the model design (e.g., network architecture).We usually achieve this by introducing inductive biases guided by the physical prior into the hypothesis space
  - Objective: we could design better loss functions or regularization terms using given physical priors like ODE/PDE/SDEs
  - Optimizer: we could design better optimization methods that are more stable or converge faster.
  - Inference: we could enforce the physical constraints by using modifying the inference algorithms.

Physics-informed machine learning

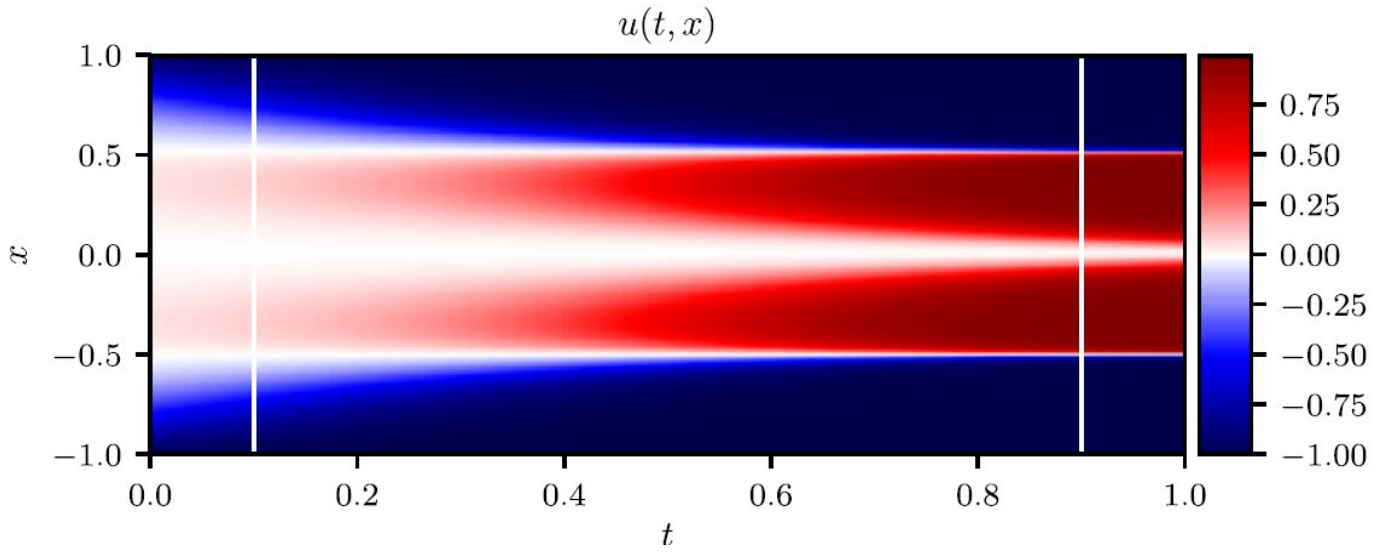
- A general form of PDEs

$$u_t(x,t) + g[u(x,t)] = 0 \quad x \in \Omega, t \in [0,T]$$

$u_t(x,t)$ denote a spatial-temporal function of the solution and g[.] is a nonlinear differential operator.

- Loss function formulation

$$L = \frac{\lambda}{|\Omega|}\int |f(u_w;\theta)(x,t)|^2 dx\,dt + \frac{\lambda}{|\Omega_0|}\int |I(u_w;\theta)(x,t)|^2 dx\,dt$$
$$+\frac{\lambda}{|\partial\Omega|}\int |B(u_w;\theta)(x,t)|^2 dx\,dt + \frac{\lambda}{N}\sum_{i=1}^{N}|u_w(x_i,t_i) - u(x_i,t_i)|^2$$


$u(t, x)$
1.0
0.5
0.0
−0.5
−1.0
x
0.0
0.2
0.4
0.6
0.8
1.0
t
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00